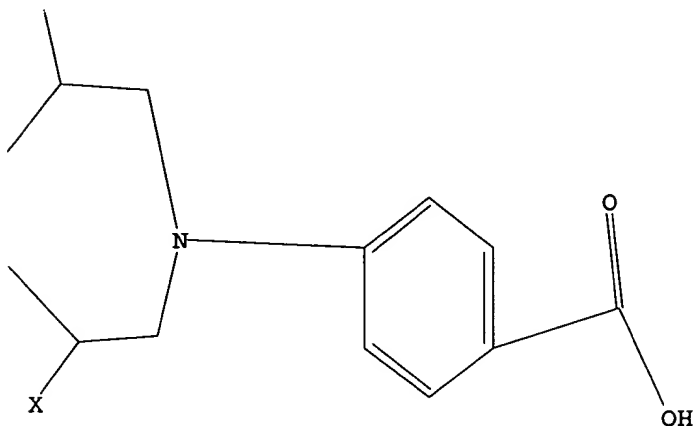


This file contains CAS Registry Numbers for easy and accurate substance identification.

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Uploading C:\STNEXP4\QUERIES\714a.str

L1        STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1        STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full  
REGISTRY INITIATED  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 19:12:26 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 708 TO ITERATE

100.0% PROCESSED        708 ITERATIONS                    2 ANSWERS  
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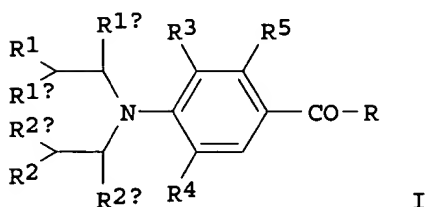
L3                    7 L2

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L3    ANSWER 1 OF 7    CAPLUS    COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER:        2000:707131    CAPLUS  
DOCUMENT NUMBER:        133:267154  
TITLE:                    Preparation of nitrogen mustard compounds and prodrugs  
INVENTOR(S):              Springer, Caroline Joy; Davies, Lawrence Christopher  
PATENT ASSIGNEE(S):        Cancer Research Campaign Technology Limited, UK  
SOURCE:                    PCT Int. Appl., 73 pp.  
                             CODEN: PIXXD2  
DOCUMENT TYPE:            Patent  
LANGUAGE:                  English  
FAMILY ACC. NUM. COUNT:    1

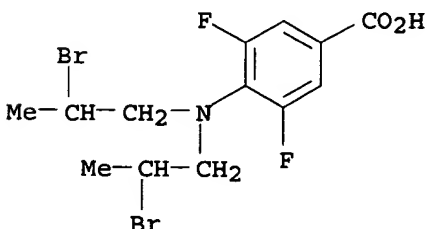
PATENT INFORMATION:

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WO 2000058271	A1	20001005	WO 2000-GB1194	20000329
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AU 2000039746	A5	20001016	AU 2000-39746	20000329
NZ 513759	A	20010928	NZ 2000-513759	20000329
EP 1165493	A1	20020102	EP 2000-918981	20000329
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JP 2002540186	T2	20021126	JP 2000-607975	20000329
PRIORITY APPLN. INFO.:			GB 1999-7414	A 19990331
			WO 2000-GB1194	W 20000329
OTHER SOURCE(S): MARPAT 133:267154				
GI				



AB Nitrogen mustard compds. and prodrugs I [R = OH or NHCH(Z)CO<sub>2</sub>R<sub>7</sub>, resp., where R<sub>1</sub>, R<sub>2</sub> = Cl, Br, I, OSO<sub>2</sub>Me, or OSO<sub>2</sub>Ph; R<sub>1a</sub>, R<sub>2a</sub>, R<sub>1b</sub>, R<sub>2b</sub> = H, Cl-4-alkyl or -haloalkyl; R<sub>3</sub> = F, Cl, Br, I, OCHF<sub>2</sub>, C.tplbond.CH, OCF<sub>3</sub>, Me, CF<sub>3</sub>, SF<sub>5</sub>, SCF<sub>3</sub>, or CF<sub>2</sub>CF<sub>3</sub>; R<sub>4</sub> = H, any group given for R<sub>3</sub>; R<sub>5</sub> = H, F; R<sub>7</sub> = H, Me<sub>3</sub>C, allyl; Z = (un)substituted -CH<sub>2</sub>-T-W, where T = CH<sub>2</sub>, O, S, S(O), or SO<sub>2</sub>; W = CO<sub>2</sub>H, CONH<sub>2</sub>, SO<sub>2</sub>NH<sub>2</sub>, SO<sub>3</sub>H, PO<sub>3</sub>H<sub>2</sub>, tetrazol-5-yl, heterocyclylthio, etc. (with provisos)] were prepared for use in therapy and treatment, for example, of cancer. Thus, [3,5-difluoro-4-[bis(2-iodoethyl)amino]benzoyl]-L-glutamic acid, prepared via amidation of 3,5-difluoro-4-[bis(2-iodoethyl)amino]benzoic acid with di-tert-butyl-L-glutamate hydrochloride, showed antitumor activity against breast carcinoma in mice at 0.98 mM vs. 2.9 mM for the prior art compound [3-fluoro-4-[bis(2-chloroethyl)amino]benzoyl]-L-glutamic acid.

IT **298211-31-1P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of nitrogen mustard compds. and prodrugs)  
 RN 298211-31-1 CAPLUS  
 CN Benzoic acid, 4-[bis(2-bromopropyl)amino]-3,5-difluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:167816 CAPLUS

DOCUMENT NUMBER: 90:167816

TITLE: Some physicochemical properties and reactivity of p-[bis(2-chloroalkyl)amino]phenylalkanoic acids

AUTHOR(S): Karpavicius, K.; Juodvirsis, A.; Prasmickiene, G.; Knunyants, I. L.

CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1979), (1), 51-8  
CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Russian

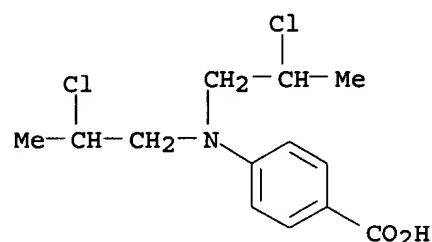
AB In p-(ClCHRCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>H (I; R = H, Me; n = 0-3) the cytotoxic amino groups exhibit an appreciable electron-donating effect, whereas the carboxyalkyl groups show a weaker effect. The CH<sub>2</sub> protons in the amino group of I (R = H; n = 1-3) are magnetically equivalent; those in I (R = H; n = 0) and the analogous cinnamic acid derivs. are not. The hydrolysis of C-Cl in I appears to be 1st order; that of I (R = Me) is an order of magnitude faster than that of I (R = H).

IT 5379-46-4

RL: PRP (Properties)  
(NMR of)

RN 5379-46-4 CAPLUS

CN Benzoic acid, 4-[bis(2-chloropropyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:58444 CAPLUS

DOCUMENT NUMBER: 88:58444

TITLE: Physicochemical properties and antileukemia activity of some p-[bis(2-chloropropyl)amino]- and p-[bis(2-chloroethyl)amino]phenylalkanoic acid derivatives

AUTHOR(S): Karpavicius, K.; Prasmickiene, G.; Juodvirsis, A.; Ivanova, L. E.; Khomchenovskii, E. I.

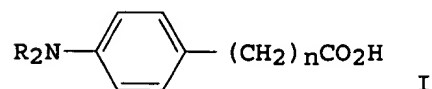
CORPORATE SOURCE: Inst. Biokhim., Vilnius, USSR

SOURCE: Poiski Izuch. Protivoopukholevykh, Protivovospalitel'nykh Mutagennykh Veshchestv (1977), 66-75. Editor(s): Kanopkaite, S. Akad. Nauk Lit. SSR, Inst. Biokhim.: Vilnius, USSR.  
CODEN: 37BOA3

DOCUMENT TYPE: Conference

LANGUAGE: Russian

GI



AB The rate of hydrolysis, pKa, PMR spectra, LD50, and antileukemic effects

of 8 p-[bis(2-chloroalkyl)amino]phenylalkanoic acids (I) were presented. The 2-chloropropyl derivs. had a greater reactive capacity than did the 2-chloroethyl derivs. owing to the presence of the electron-donor Me group. The 2-chloropropyl derivs. were also generally more toxic than the 2-chloroethyl groups. The 2-chloropropyl derivs. were effective against granulocytopenias and on transplanted leukemias Nk/Ly and L-1210 in mice, whereas the 2-chloroethyl derivs. were effective against lymphopoiesis and development of Shchvetz leukemia in rats.

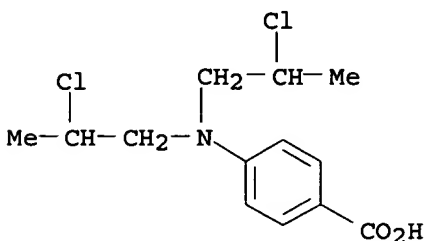
IT 5379-46-4

RL: BIOL (Biological study)

(antileukemic activity and physicochem. properties of)

RN 5379-46-4 CAPLUS

CN Benzoic acid, 4-[bis(2-chloropropyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:15944 CAPLUS

DOCUMENT NUMBER: 88:15944

TITLE: Comparative study of the general toxicity and antileukemic activity of new phenylalkanoic acid derivatives under experimental conditions

AUTHOR(S): Ivanova, L. E.; Zaretskii, I. I.; Khomchenovskii, E. I.; Karpavicius, K.; Prasmickiens, G.

CORPORATE SOURCE: Moscow, USSR

SOURCE: Leikozologiya (1975), 4, 23-9

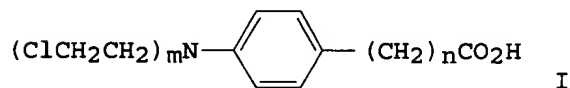
CODEN: LEIKDK

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

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AB The toxicity and antileukemic effects of 8 phenylalkanoic acids (I) were determined. The 2-chloropropyl derivs., p-di(2-chloropropyl)aminobenzoic acid [5379-46-4], p-di(2-dichloropropyl)aminophenylacetic acid [19521-09-6], p-di(2-chloropropyl)aminophenylpropionic acid [22812-54-0], and p-di(2-chloropropyl)aminophenylbutyric acid [55774-31-7] had greater antileukemic effects than the resp. 2-chloroethyl derivs. although LD50 values tended to be lower.

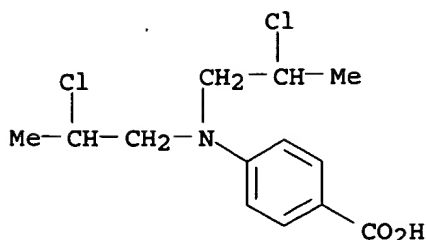
IT 5379-46-4

RL: BIOL (Biological study)

(leukemia inhibition by)

RN 5379-46-4 CAPLUS

CN Benzoic acid, 4-[bis(2-chloropropyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:430178 CAPLUS

DOCUMENT NUMBER: 71:30178

TITLE: Synthesis and study of the reactivity of  
p-[bis(2-chloropropyl)amino]phenylalkanoic acids

AUTHOR(S): Prasmickiene, G.; Sukeliene, D.; Karpavicius, K.;  
Kil'disheva, O. V.

CORPORATE SOURCE: Nauch.-Issled. Inst. Onkol., Vilnius, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya  
(1969), (3), 643-6  
CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Russian

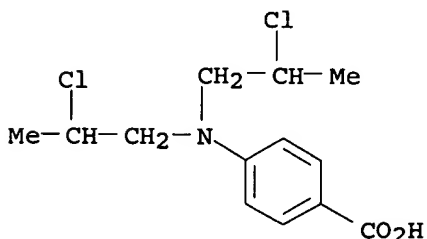
AB To 2.2 ml. POCl<sub>3</sub> in Me<sub>2</sub>NCHO was added 5.72 g. p-(ClCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> in the same solvent and the mixture kept 1 day at 40° to give p-(ClCH-MeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO, (I), m. 104-6°. I with N<sub>2</sub>H<sub>4</sub> gave the appropriate ylidenehydrazine, m. 167-9°, while HONH<sub>2</sub> gave the oxime, m. 125-7°, which after 3 hrs. reflux in Ac<sub>2</sub>O gave 71% p-(ClCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN, m. 128-30°, which heated in concentrated H<sub>2</sub>SO<sub>4</sub> 2 hrs. at 50° gave the corresponding amide, m. 138-40°. Oxidation of the aldehyde or heating the benzamide with HCl gave p-(ClCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, m. 160-2°. Propylene oxide added to p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CH<sub>2</sub>CONH<sub>2</sub> in 30% AcOH gave, in 1 day, 77% (HOCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CH<sub>2</sub>CONH<sub>2</sub>, m. 102-4°, which, heated with POCl<sub>3</sub> 1 hr., gave, on quenching in ice, 73% p-(ClCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CH<sub>2</sub>CN (II), m. 66-8°, which in concentrated H<sub>2</sub>SO<sub>4</sub> 2 hrs. at 50° gave the corresponding amide, m. 58-60°. I heated with malonic acid in pyridine-piperidine 3 hrs. gave 76% p-(ClCHMeCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH:CHCO<sub>2</sub>H (III), m. 131-3°. II heated with concentrated HCl gave 59% corresponding free acid, m. 69-71°, also formed by hydrogenation of III over PdCaCO<sub>3</sub>.

IT 5379-46-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 5379-46-4 CAPLUS

CN Benzoic acid, 4-[bis(2-chloropropyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:84288 CAPLUS

DOCUMENT NUMBER: 64:84288

ORIGINAL REFERENCE NO.: 64:15785d-g

TITLE: Tumor chemotherapy. XXX. Studies on the  
hexamethylenetetramine salt of p-bis(2-  
chloroethyl)amino-ω-bromoacetophenone

AUTHOR(S): Jen, Yun-Feng; Kao, I-Sheng

CORPORATE SOURCE: Inst. Mater. Med., Acad. Sinica, Shanghai, Peop. Rep. China

SOURCE: Huaxue Xuebao (1965), 31(6), 486-92,500  
CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal

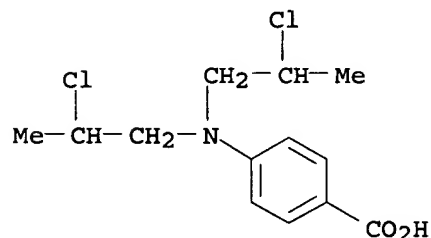
LANGUAGE: Chinese

AB cf. CA 63, 17000b. p-(XRCHCH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>[(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>]+Br- (Ia) (X = Br, R = H) (I), (X = I, R = H) (II), p-EtO<sub>2</sub>CNHC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>[(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>]+Br- (III), and p-EtO<sub>2</sub>CNHC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>SC(:NH<sub>2</sub>+Br-)NH<sub>2</sub> (IV), the analogs of the antitumor compound AT-584, were prepared. The starting materials for the synthesis of I and II were p-bis[2-haloethyl (and propyl)] aminobenzoic acids (V and VI), resp. VI was synthesized by 2 methods: (1) [R(HO)CHCH<sub>2</sub>]<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et-p was first halogenated with PBr<sub>3</sub> or POCl<sub>3</sub> and then hydrolyzed with HCl or HBr to yield p-bis[2-chloropropyl (and 2-bromoethyl)] aminobenzoic acids. (2) Chlorination of p-bis(2-hydroxypropyl)aminobenzene with POCl<sub>3</sub> in dimethylformamide gave p-bis(2-chloropropyl)aminobenzaldehyde, which was treated with KMnO<sub>4</sub> in acetone to afford VI. The 2nd route gave a better yield. V and VI in benzene reacted sep. with SOCl<sub>2</sub> to give the acid chlorides, which were treated sep. with diazomethane to yield the diazoacetophenones (VII). VII were decomposed in dioxane with HBr to form bromoacetophenone derivs., which treated with hexamethylenetetramine in chloroform gave I and II, resp. p-Aminoacetophenone was treated with ethyl chloroformate in the presence of triethylamine as the condensing agent to form p-ethoxycarbonyliminoacetophenone (VIII). When N,N-diethylaniline was used as the condensing agent instead of triethylamine, the yield was better. VIII was first brominated in acetic acid with Br and then treated with hexamethylenetetramine or thiourea to afford III and IV, resp. Preliminary pharmacol. examns. showed that I and II were as active as AT-584 against HeLa cells in culture medium, while III and IV were less active.

IT 5379-46-4, Benzoic acid, p-[bis(2-chloropropyl)amino]- (preparation of)

RN 5379-46-4 CAPLUS

CN Benzoic acid, 4-[bis(2-chloropropyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1951:863 CAPLUS

DOCUMENT NUMBER: 45:863

ORIGINAL REFERENCE NO.: 45:139h-i,140a-g

TITLE: Aryl-2-haloalkylamines. VII. Some derivatives of 2-naphthyldi(2-haloalkylamines)

AUTHOR(S): Davis, W.; Everett, J. L.; Ross, W. C. J.

CORPORATE SOURCE: Roy. Cancer Hosp., London

SOURCE: Journal of the Chemical Society, Abstracts (1950) 1331-7  
CODEN: JCSAAZ; ISSN: 0590-9791

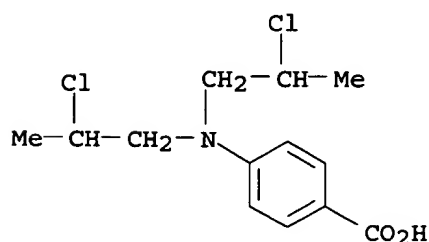
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 44, 6838i. This work is a continuation of that in C.A. 43, 7442g, and 44, 1431e, in which it was shown that many arylbis(2-haloalkyl)amines inhibited the growth of various animal tumors and of spontaneous and transmitted leukemia in the Furth AK 1 pure line; 2-C<sub>10</sub>H<sub>7</sub>N(CH<sub>2</sub>CH<sub>2</sub>Cl)<sub>2</sub> has been used clinically for the treatment of various lymphadenopathies in human patients with encouraging results. 1,7-AcC<sub>10</sub>H<sub>6</sub>NH<sub>2</sub> (16 g.), added to 11.2 g. NaOH and 18.4 g. 50% N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O in 175 g. (HOC<sub>2</sub>H<sub>4</sub>)<sub>2</sub>O and heated 3 hrs. at 195°, gives 14.5 g.

1,7-EtCl<sub>10</sub>H<sub>6</sub>NH<sub>2</sub>, brown oil (Ac derivative, m. 167°).  
 1,2,3,4-Tetrahydronaphthalene (264 g.), nitrated according to Schroeter (C.A. 16, 1673), gives 60 g. 5-NO<sub>2</sub> and 45 g. 6-NO<sub>2</sub> derivs.; catalytic reduction (Raney Ni) gives 5,6,7,8-tetrahydro-1- and -2-naphthylamines. 1-Keto-1,2,3,4-tetrahydronaphthalene oxime, reduced with Na in EtOH, gives 1,2,3,4-tetrahydro-1-naphthylamine, b<sub>10</sub> 114°. These amines were converted into the N,N-bis(2-hydroxyethyl) derivs. in the usual manner but it is preferable to use SOCl<sub>2</sub> in CHCl<sub>3</sub> for the chlorination stage, N,N-Bis(2-chloroethyl)-2-methyl-1-naphthylamine, oil.  
 1,2,3,4-Tetrahydro-N,N-bis(2-hydroxyethyl)-1-naphthylamine, m. 89° (picrate, m. 140°); N,N-bis-(2-chloroethyl)-1,2,3,4-tetrahydro-1-naphthylamine-HCl, m. 158°. 5,6,7,8-Tetrahydro-N,N-bis(2-hydroxyethyl)-1-naphthylamine picrate, m. 199° (decomposition); N,N-bis(2-chloroethyl)-5,6,7,8-tetrahydro-1-naphthylamine, an oil (picrate, m. 121°). N-(2-Naphthyl)-N-methyl-2-hydroxyethylamine picrate, m. 160°; N-(2-naphthyl)-N-methyl-2-chloroethylamine, m. 52.5° (inactive); N-(2-naphthyl)-N-methyl-2-hydroxypropylamine picrate, m. 154°; N-(2-naphthyl)-N-methyl-2-chloropropylamine, m. 64° (inactive). N,N-bis(2-hydroxyethyl)-6-methyl-2-naphthylamine, m. 94°; N,N-bis(2-chloroethyl)-6-methyl-2-naphthylamine, m. 65°; bis(2-bromoethyl) analog, m. 88°; bis(2-iodoethyl) analog, m. 100-1°. N,N-Bis(2-chloroethyl)-8-methyl-2-naphthylamine, m. 63°; 8-Et homolog, m. 48°; bis(2-bromoethyl)-8-ethyl analog, m. 57°; bis(2-iodoethyl) analog, m. 85°. 8-Acetyl-N,N-bis(2-hydroxyethyl)-2-naphthylamine, yellow, m. 113°; bis(2-chloroethyl) analog, yellow, m. 84°; bis(2-bromoethyl) analog, yellow, m. 94.5° (solns. of the last 2 compds. exhibit an intense yellow-green fluorescence).  
 N-(2-Chloroethyl)-1,2,3,4-tetrahydro-2-naphthylamine-HCl, m. 215°; picrate, m. 197°. N,N-Bis(2-chloroethyl)-1,2,3,4-tetrahydro-2-naphthylamine-HCl, m. 164°; bis(2-bromoethyl) analog-HBr, m. 229°. 5,6,7,8-Tetrahydro-N,N-bis(2-hydroxyethyl)-2-naphthylamine, m. 57°; bis(2-chloroethyl) analog, m. 65°, photoluminescent.  
 N,N-Bis(2-hydroxyethyl)-2-phenanthrylamine, m. 155°; bis-(2-chloroethyl) analog, m. 91-2°; bis(2-bromoethyl) analog, m. 111-12°; bis(2-iodoethyl) analog, m. 117°.  
 N,N-Bis(2-hydroxyethyl)-3-phenanthrylamine, m. 109-10°; bis(2-chloroethyl) analog, m. 73°; bis(2-bromoethyl) analog, m. 98°; bis(2-iodoethyl) analog, m. 125°. 2-(2-Hydroxyethylamino)fluorene, yellow, m. 150° (cf. C.A. 43, 7442g); 2-chloroethyl analog, m. 127°. 2-[Bis(2-bromoethyl)amino]fluorene m. 137°. N'-Propionyl-N,N-bis(2-chloroethyl)-p-phenylenediamine m. 101-3°. p-[Bis(2-chloropropyl)amino]benzoic acid, m. 165-6°; Me ester, m. 61°. p-MeOC<sub>6</sub>H<sub>4</sub>N(CH<sub>2</sub>CH<sub>2</sub>Cl)<sub>2</sub> (2.5 g.) and 3.4 g. Et<sub>2</sub>NCS<sub>2</sub>Na in 200 ml. 50% aqueous Me<sub>2</sub>CO, refluxed 2 hrs., give N,N-bis[2-(diethyldithiocarbamyl)ethyl]-p-anisidine, m. 85-6°. p-MeOC<sub>6</sub>H<sub>4</sub>[NCH<sub>2</sub>CH(OH)CH<sub>2</sub>Cl]<sub>2</sub> (40 g.) in 500 ml. boiling ether, gradually treated with 40 g. KOH, gives N,N-bis(2,3-epoxypropyl)-p-anisidine, yellow, b<sub>9</sub> 228-9°; this is inactive. Data are given for the rate of hydrolysis of a number of these compds. in 50% aqueous Me<sub>2</sub>CO at 66°. The effect of various substituents is discussed. There is the expected increase in the rate of hydrolysis on passing from the Cl to Br compound but a somewhat surprising decrease for the iodides.

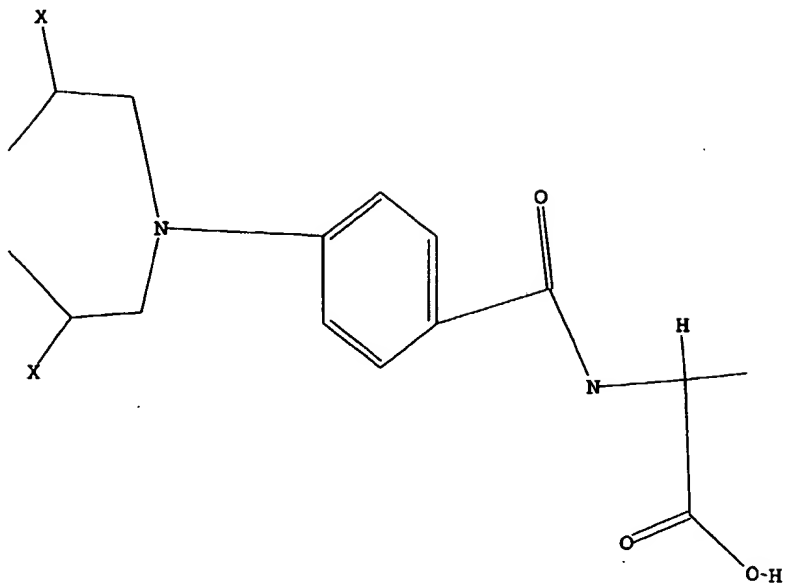
IT 5379-46-4, Benzoic acid, p-[bis(2-chloropropyl)amino]-(preparation of)  
 RN 5379-46-4 CAPLUS  
 CN Benzoic acid, 4-[bis(2-chloropropyl)amino]-(9CI) (CA INDEX NAME)



=>  
Uploading 714.str

L1        STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1        STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1  
REGISTRY INITIATED  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 10:55:44 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -        2 TO ITERATE

100.0% PROCESSED        2 ITERATIONS        0 ANSWERS  
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                             BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        2 TO        124  
PROJECTED ANSWERS:            0 TO        0

L2        0 SEA SSS SAM L1

L3        0 L2

=> s l1 full  
REGISTRY INITIATED  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 10:55:52 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS  
SEARCH TIME: 00.00.02

1 ANSWERS

L4 1 SEA SSS FUL L1

L5 1 L4

=> d ibib abs hitstr

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:707131 CAPLUS

DOCUMENT NUMBER: 133:267154

TITLE: Preparation of nitrogen mustard compounds and prodrugs

INVENTOR(S): Springer, Caroline Joy; Davies, Lawrence Christopher

PATENT ASSIGNEE(S): Cancer Research Campaign Technology Limited, UK

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

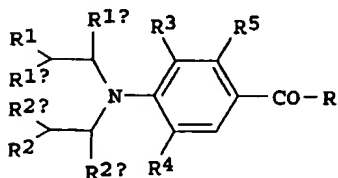
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000058271	A1	20001005	WO 2000-GB1194	20000329
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
NZ 513759	A	20010928	NZ 2000-513759	20000329
EP 1165493	A1	20020102	EP 2000-918981	20000329
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002540186	T2	20021126	JP 2000-607975	20000329
PRIORITY APPLN. INFO.:			GB 1999-7414	A 19990331
			WO 2000-GB1194	W 20000329
OTHER SOURCE(S):		MARPAT 133:267154		
GI				



AB Nitrogen mustard compds. and prodrugs I [R = OH or NHCH(Z)CO2R7, resp., where R1, R2 = Cl, Br, I, OSO2Me, or OSO2Ph; R1a, R2a, R1b, R2b = H,

Cl-4-alkyl or -haloalkyl; R3 = F, Cl, Br, I, OCHF2, C.tplbond.CH, OCF3, Me, CF3, SF5, SCF3, or CF2CF3; R4 = H, any group given for R3; R5 = H, F; R7 = H, Me3C, allyl; Z = (un)substituted -CH2-T-W, where T = CH2, O, S, S(O), or SO2; W = CO2H, CONH2, SO2NH2, SO3H, PO3H2, tetrazol-5-yl, heterocyclylthio, etc. (with provisos)] were prepd. for use in therapy and treatment, for example, of cancer. Thus, [3,5-difluoro-4-[bis(2-iodoethyl)amino]benzoyl]-L-glutamic acid, prepd. via amidation of 3,5-difluoro-4-[bis(2-iodoethyl)amino]benzoic acid with di-tert-butyl-L-glutamate hydrochloride, showed antitumor activity against breast carcinoma in mice at 0.98 mM vs. 2.9 mM for the prior art compd. [3-fluoro-4-[bis(2-chloroethyl)amino]benzoyl]-L-glutamic acid.

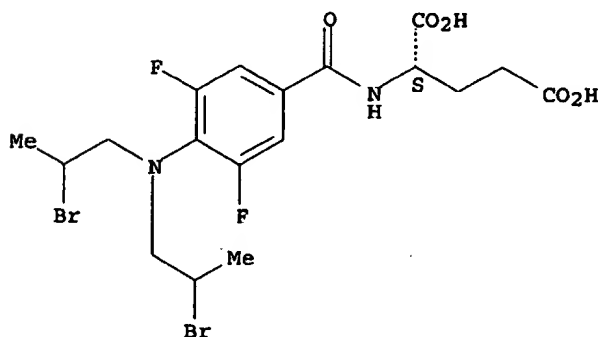
IT 298211-06-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of nitrogen mustard compds. and prodrugs)

RN 298211-06-0 CAPLUS

CN L-Glutamic acid, N-[4-[bis(2-bromopropyl)amino]-3,5-difluorobenzoyl]-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

1/1

Figure 1A

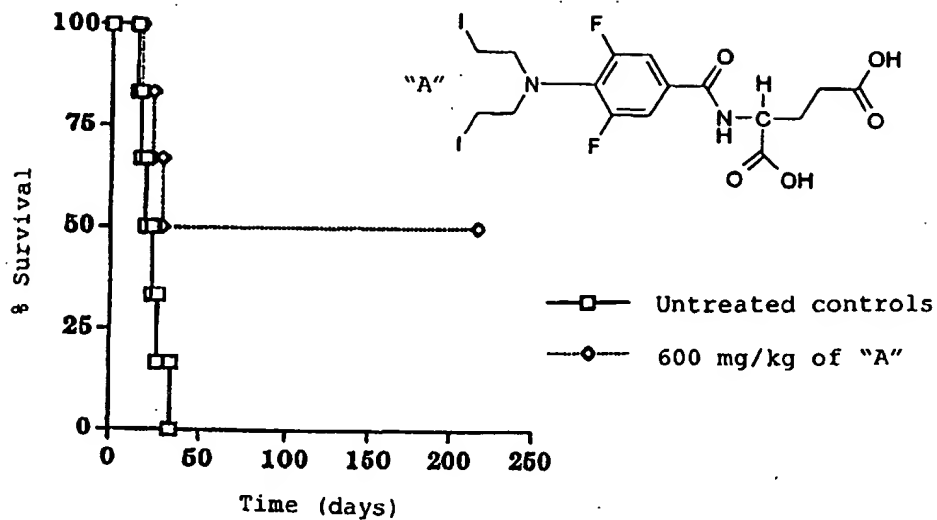


Figure 1B

